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Exact Solution for Contaminant Transport with Nonlinear Sorption

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Abstract—We study a contaminant transport model with a cubic approximation for Langmuir sorption. It is shown that the aqueous concentration profile can be obtained exactly in the form of a traveling wave front. We outline the methodology of obtaining the exact solution and present two possible closed form solutions.

Keywords—Contaminant transport, Traveling wave, Heteroclinic orbit, Exact solution, Direct algebraic method.

1. INTRODUCTION

In the study of contamination of groundwater, researchers often use transport models along with sorption equations to assess the risk of contamination and devise remedial strategies. Since such models are nonlinear, most of the studies to date have been computational. We show that, under certain conditions, it is possible to obtain the exact closed form solution of a nonlinear contaminant transport model. As noted in [1], an exact solution can provide a better insight into the effects of physical and chemical processes on solute transport compared to any numerical solution of a given model. The exact solution, which is a traveling wave front, is obtained using simple and nonsophisticated mathematical techniques. However, it should be pointed out that the same solution can also be found employing the direct algebraic method of Hereman *et al.* [2] which formulates the solution as an infinite series of harmonics of the real exponential solutions of the associated linear system.

2. CONTAMINANT TRANSPORT MODEL AND EXACT SOLUTIONS

Let us consider the contaminant transport model in the following nondimensional form:

$$c_t = \frac{1}{P} c_{xx} - c_x - \omega q_t, \tag{2.1}$$

$$q_t = L\left[f(c) - q\right], \qquad -\infty < x < \infty, \quad t > 0, \tag{2.2}$$

where c and q are the concentrations of the solute in the aqueous phase and the adsorbed phase, respectively. The constants P, L and w are positive, and they are functions of porosity, bulk density and pore-water velocity.

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In practice, the adsorption isotherm $f(c)$ is assumed to be either Langmuir or Freundlich isotherm [3–6]. However, for low solute concentrations, the Langmuir isotherm can be viewed as a cubic isotherm such as

$$f(c) = KQc\left(\alpha - Kc + K^2c^2\right). \tag{2.3}$$

For the work presented in this paper, we chose $f(c)$ as in (2.3) with appropriate positive values for the constants α, K and Q.

We study the problem with the following conditions:

$$\lim_{x\to-\infty} c(x,t) = 0, \qquad c(x,t) > 0, \qquad \lim_{x\to-\infty} \frac{\partial}{\partial x} c(x,t) = 0, \quad \text{and} \quad \lim_{x\to-\infty} q(x,t) = 0.$$

Introducing the traveling wave coordinate $z = x - vt$, where v is the constant speed at which the wave is assumed to be moving, we obtain a coupled system of ordinary differential equations with respect to z,

$$-vc' = \frac{1}{P}c'' - c' + v\omega q', \tag{2.4}$$

$$-vq' = L\left[f(c) - q\right]. \tag{2.5}$$

After a few simple mathematical operations, the coupled system of ordinary differential equations can be reduced to a single second order differential equation in c such as

$$c'' - \left[\frac{L}{v} + P(1-v)\right] c' + LP\omega K^2Qc^2 - LP\omega K^3Qc^3 - LP\left(\alpha\omega KQ + 1 - \frac{1}{v}\right)c = 0. \tag{2.6}$$

Now, by letting $x_1 = c$ and $x_2 = c'$, (2.6) can be rewritten as

$$\begin{aligned} x_1' &= x_2, \\ x_2' &= Ax_1 - Bx_1^2 + Ex_1^3 + \epsilon x_2. \end{aligned} \tag{2.7}$$

Here,

$$A = LP\left(\alpha\omega KQ + 1 - \frac{1}{v}\right), \quad B = LP\omega K^2Q, \quad E = LP\omega K^3Q, \quad \text{and} \quad \epsilon = \frac{L}{v} + P(1-v).$$

When $\epsilon = 0$, (2.7) will have three equilibrium points, provided that $B^2 - 4AE > 0$, and the integration of the system will give us

$$x_2^2 = \left(A - \frac{2}{3}Bx_1 + \frac{1}{2}Ex_1^2\right)x_1^2. \tag{2.8}$$

The right-hand side of (2.8) is either positive or zero, if

$$B^2 \le \frac{9}{2}AE.$$

Let us consider the case,

$$B^2 = \frac{9}{2}AE, \tag{2.9}$$

which corresponds to choosing the constant α such that

$$\alpha = \frac{v(2\omega KQ - 9) + 9}{9v\omega KQ}. \tag{2.10}$$

For this choice of α, the three equilibrium points of (2.7), with $\epsilon = 0$, are $p_0 = (0,0)$, $p_1 = (1/3K, 0)$ and $p_2 = (2/3K, 0)$. It can be easily verified that p_0 and p_2 are hyperbolic saddle points while p_1 is a center. The associated phase plane diagram for this case is given in Figure 1.

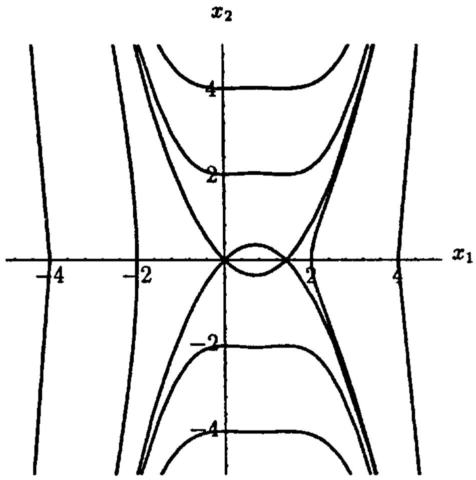

Figure 1. Phase plane portrait of the equation (2.7) with $A = 1$, $E = 1$, $\epsilon = 0$ and B satisfying (2.9). The figure shows the heteroclinic orbit defined by (2.11), which corresponds to the wave front solution for the aqueous concentration.

Further, from (2.8) we can write down

$$x_2 = \pm\sqrt{\frac{E}{2}}\left(x_1 - \frac{2}{3K}\right)x_1. \tag{2.11}$$

Since we have the condition $\lim_{x\to-\infty} c(x,t) = 0$, the nondecreasing solution will be found when

$$x_2 = -\sqrt{\frac{E}{2}}\left(x_1 - \frac{2}{3K}\right)x_1, \qquad 0 \le x_1 \le \frac{2}{3K}. \tag{2.12}$$

Integration of (2.12) will give this solution as

$$x_1 = c = \frac{2}{3K\left(1 + e^{-(2/3K)\sqrt{E/2}\,(z+x_0)}\right)};$$

i.e.,

$$c(x,t) = \frac{2}{3K\left(1 + e^{-(2/3K)\sqrt{E/2}\,(x-vt+x_0)}\right)}, \tag{2.13}$$

which is a traveling wave front. The constant x_0 relates to the initial position of the front. Note that taking the plus sign in (2.11) will give a physically meaningless solution for aqueous concentration. However, if we impose the conditions

$$\lim_{x\to\infty} c(x,t) = 0 \quad \text{and} \quad \lim_{x\to\infty} q(x,t) = 0$$

to the original problem (2.1) and (2.2) instead of

$$\lim_{x\to-\infty} c(x,t) = 0 \quad \text{and} \quad \lim_{x\to-\infty} q(x,t) = 0,$$

then the solution for c will be a nonincreasing wave profile. Now, taking the plus sign in (2.11), we can find this solution, and it is

$$c(x,t) = \frac{2}{3K\left(1 + e^{(2/3K)\sqrt{E/2}\,(x-vt+x_0)}\right)}. \tag{2.14}$$

Figures 2 and 3 show these profiles of c.

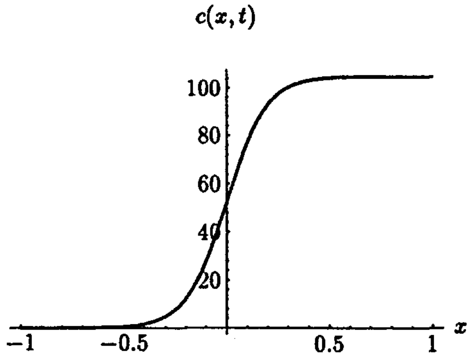

Figure 2. The nondecreasing concentration profile for aqueous concentration given by (2.13). The parameter values are $\epsilon = 0$, $\omega = 20/9$, $P = 100/3$, $L = 1000$, $Q = 1$, $K = 0.00636$ and $v = 6$.

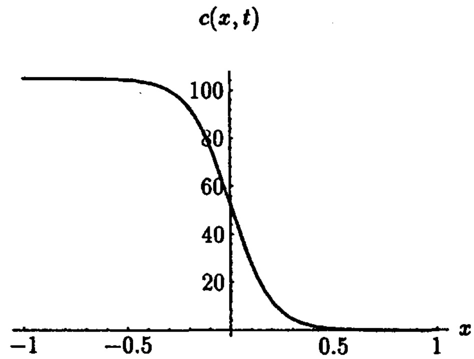

Figure 3. The nonincreasing concentration profile for aqueous concentration given by (2.14). The parameter values are $\epsilon = 0$, $\omega = 20/9$, $P = 100/3$, $L = 1000$, $Q = 1$, $K = 0.00636$ and $v = 6$.

As mentioned in the introduction, the exact solutions (2.13) and (2.14) can also be found by using the direct algebraic method of Hereman *et al.* [2]. Here, we look for a solution of the form

$$c(z) = \sum_{n=1}^{\infty} a_n \left[\exp\{-\kappa z\}\right]^n, \tag{2.15}$$

where $\exp\{-\kappa z\}$ corresponds to the solution of the associated linear equation. κ is a real function of v and, in general, a_n is a polynomial of n. For our analysis, we take a_n as

$$a_n = nA_1 + A_0. \tag{2.16}$$

Now, by simply substituting (2.15) into (2.6) and collecting the coefficients of every power of $\exp\{-\kappa z\}$ and setting each individual coefficient to zero, we obtain algebraic equations in κ, A_0 and A_1. By solving these algebraic equations with the help of the symbolic software *MATHEMATICA*, we find that $\kappa = K$ and the solutions are

$$c(x,t) = \frac{1 \pm \tanh\left\{(1/3\,K)\sqrt{E/2}\,(x - vt + x_0)\right\}}{3\,K}, \tag{2.17}$$

which are the same as those given in (2.13) and (2.14). Although our exact solutions are obtained for $\epsilon = 0$, one should note that other solutions do exist when $\epsilon \neq 0$. However, as far as we could see, these other solutions can be determined only numerically.

3. CONCLUSION

In this short paper, we have shown that certain exact solute concentration profiles can be found for contaminant transport with the appropriate nonlinear sorption. The methodology presented here can also be useful in studying other problems which exhibit traveling wave solutions.

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